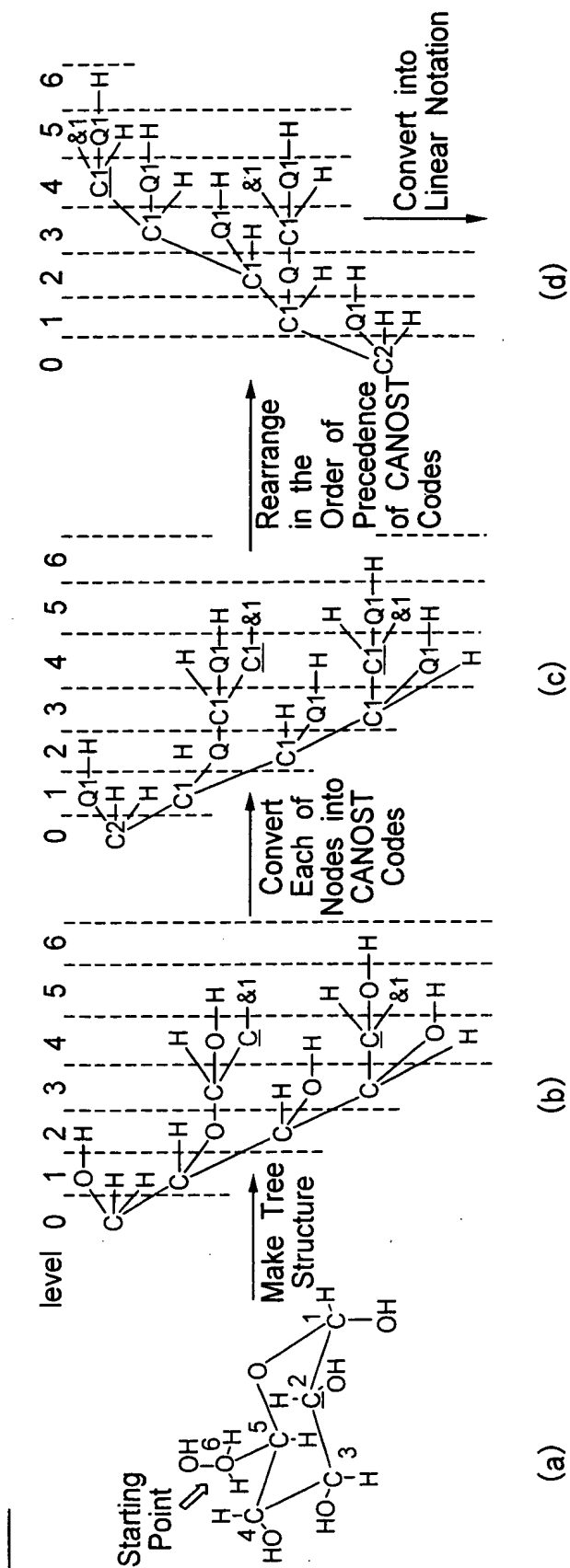


FIG. 1


$$C2 * C1; Q1; H; H * C1; Q; H, H, *, C1; Q1; H, C1, *, C1; Q1; H, H, &1; Q1; H * &1; Q1; H, H, *, H, *, *$$

(e)

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FIG. 2

Starting point (Start Atom)

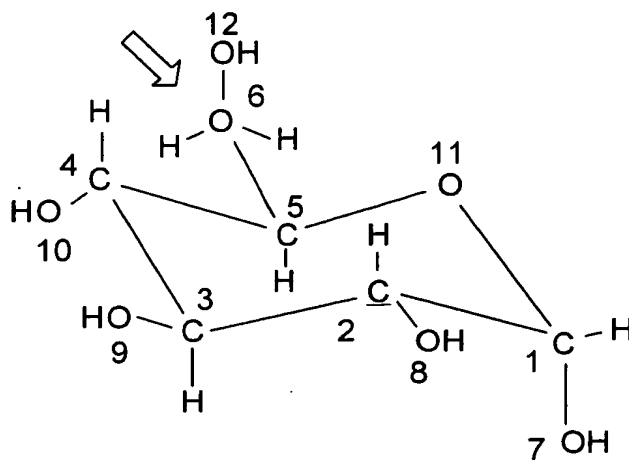
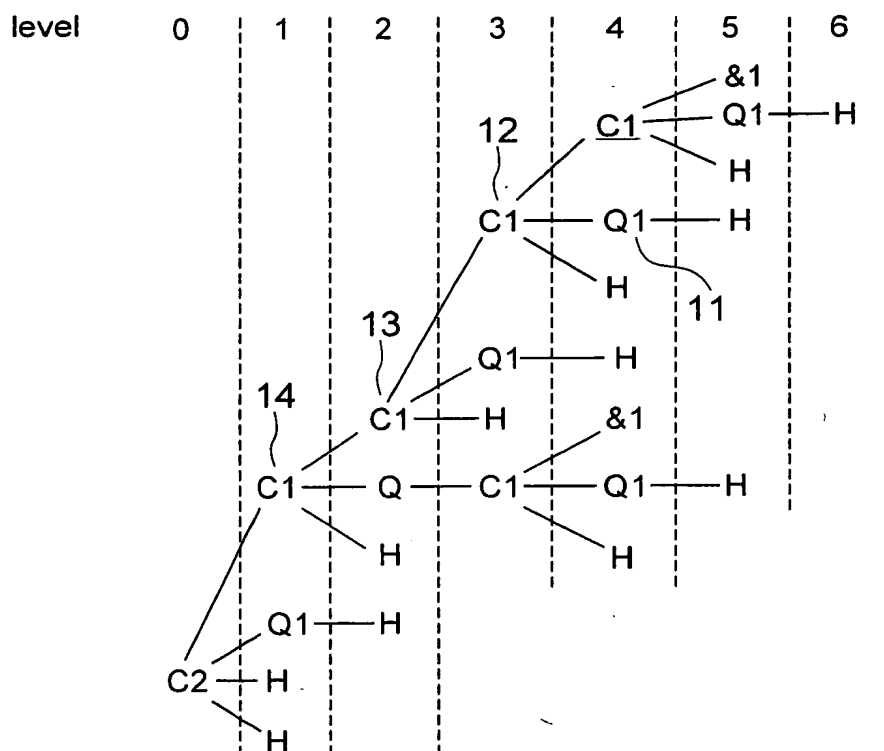


FIG. 3


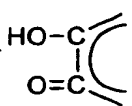

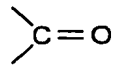

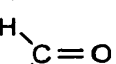









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FIG. 4

CANOST (modified) code list

no	code	substructure	no.	code	substructure	no.	code	substructure
1 ^{a)}	&nc	code for ring closing	12 ^{b)}	Y		22	LF	—F
2	T	$\text{—C}\equiv$	13 ^{c)}	Y1	$\text{H—C}\langle$	23	LC	—Cl
3	T1	$\text{H—C}\equiv$	14 ^{d)}	YTT		24	LB	—Br
4	DD	=C=				25	LJ	—I
5	DS		15	V		26	X	other atom
6	D1		16	V1		27 ^{e)}	XR	$\text{X}\langle$
7	D2		17	VD	=C=O	28	XW	
8	C		18	QD	=O	29	XD	=X
9	C1		19	Q	=O—	30	XN	=X=
10	C2		20	Q1	—O—H	31	XT	$\equiv\text{X}$
11	C3		21	Q0	—O^-	32 ^{f)}	Xnp	XH_{np}
						33	H	—H

a) A cn is a serial no. of the closing site.

b) Aromatic carbon without hydrogen.

c) Aromatic carbon with hydrogen.

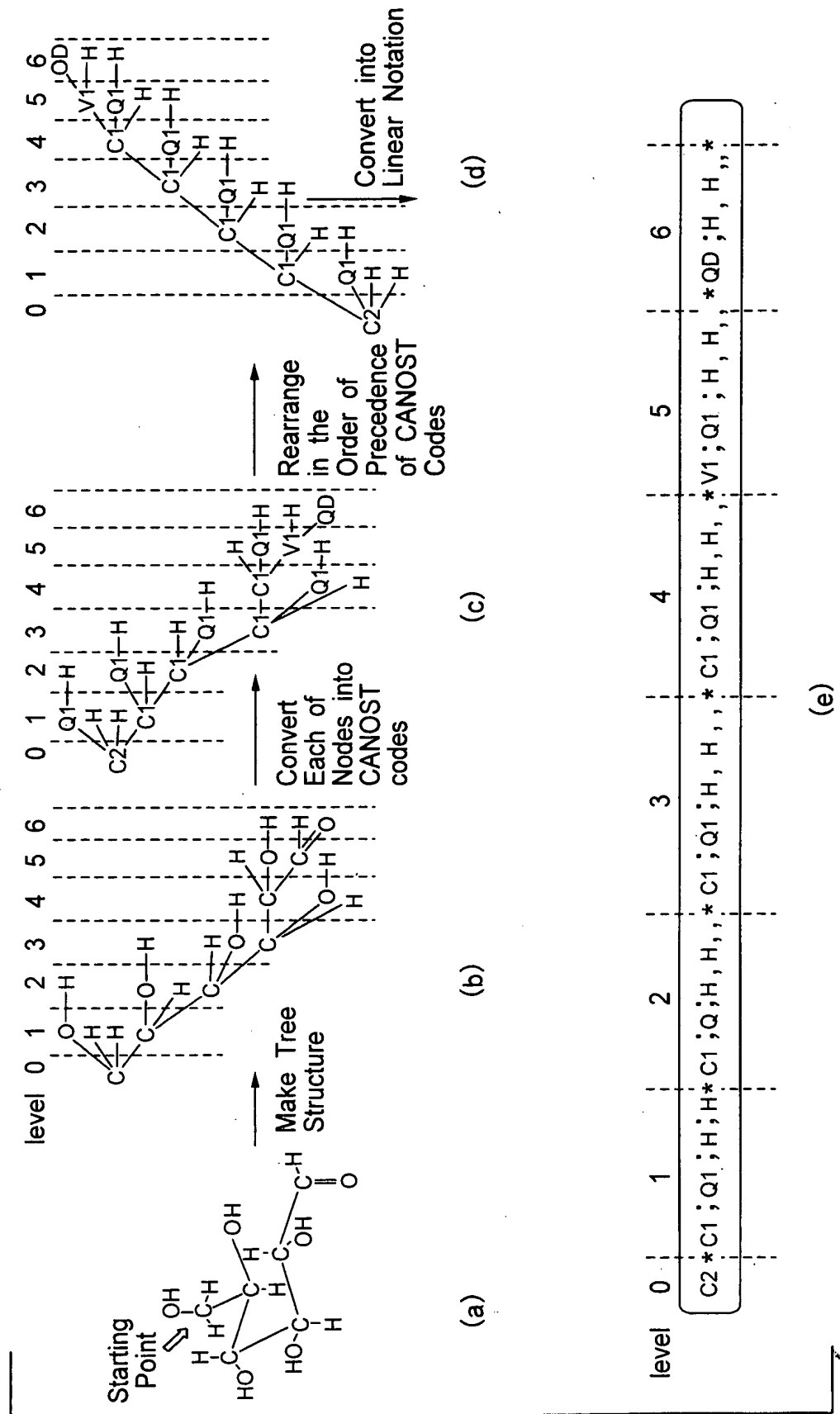
d) —C(OH)—C(O)— in troponoid.

e) Non-carbon atom in aromatic structure.

f) A np is the number of connecting hydrogens.

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FIG. 5



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FIG. 6

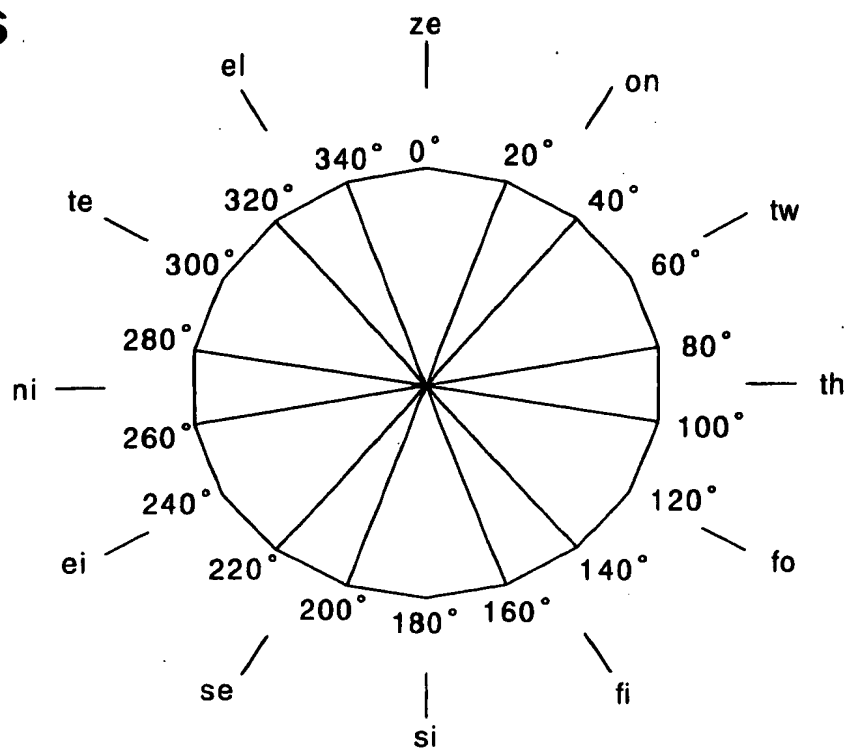
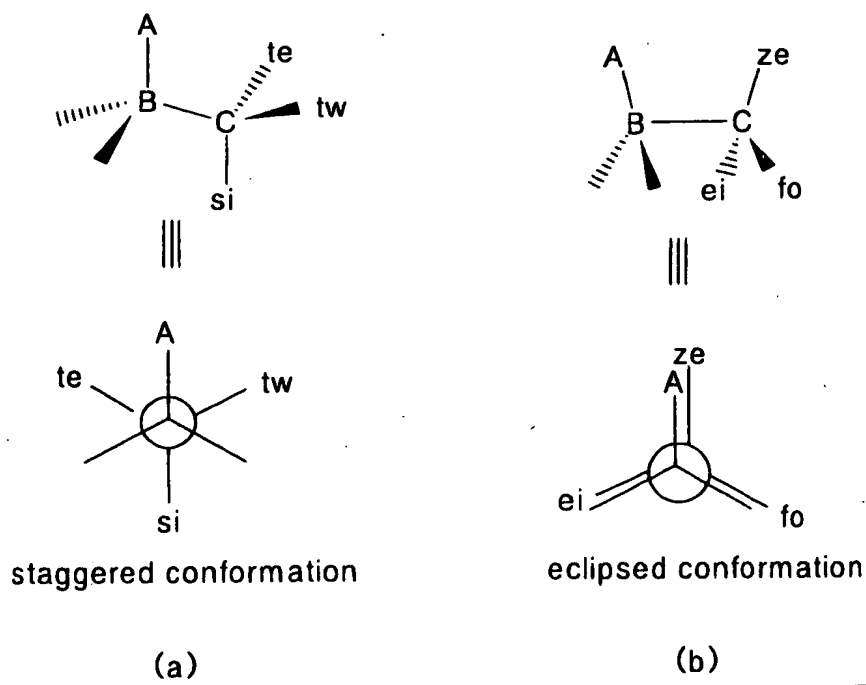
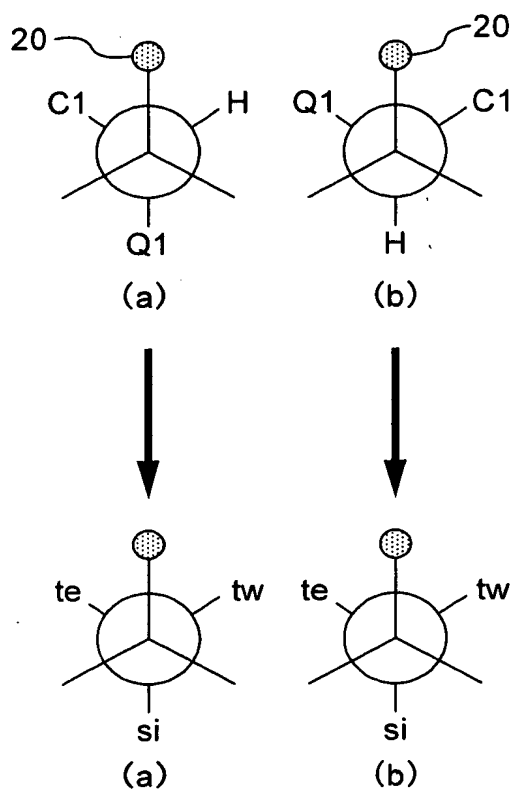


FIG. 7



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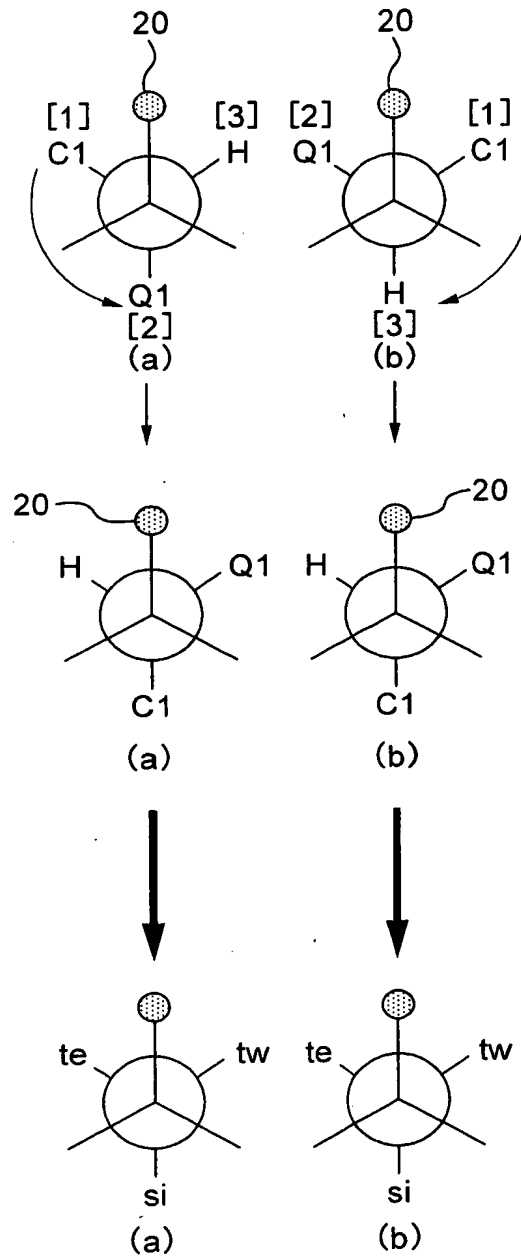
FIG. 8



CANOST Code	C1;Q1;H,
STEREO Code (a)	te;si;tw
STEREO Code (b)	tw;te;si

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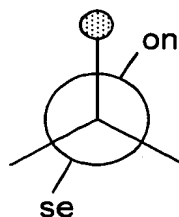
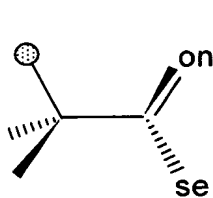
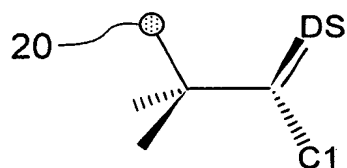
FIG. 9



CANOST Code	C1;Q1;H,
Configuration Identification Code (a)	si;tw;te
Configuration Identification Code (b)	si;tw;te

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FIG. 10

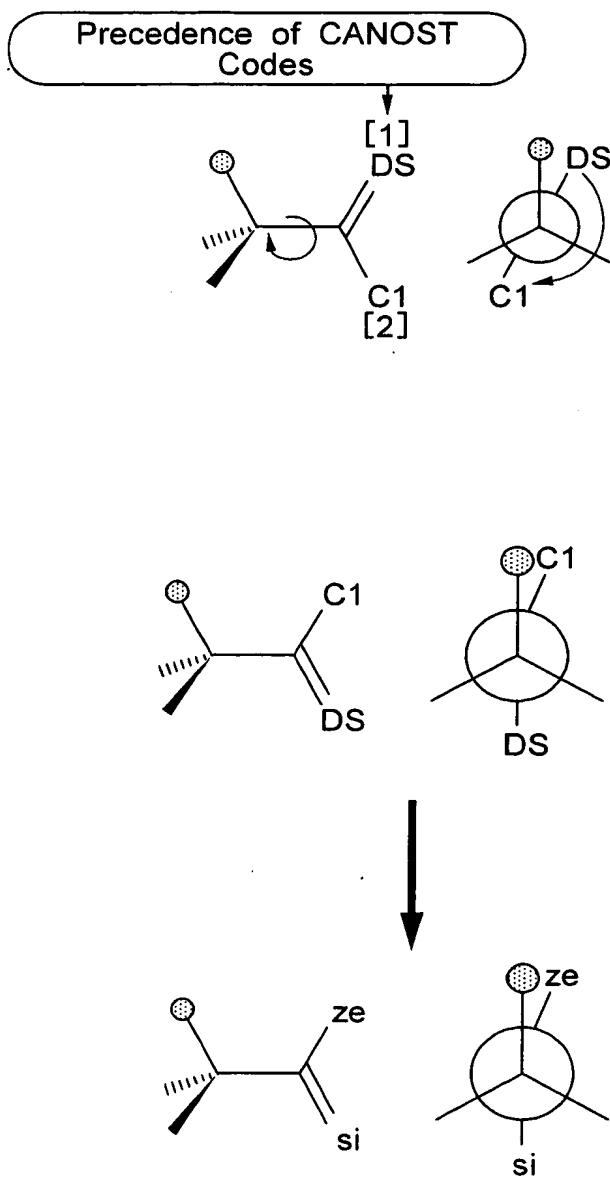


CANOST Code	DS;C1
STEREO Code	on;se

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FIG. 11.



CANOST Code	DS;C1
Configuration Identification Code	si;ze

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FIG. 12

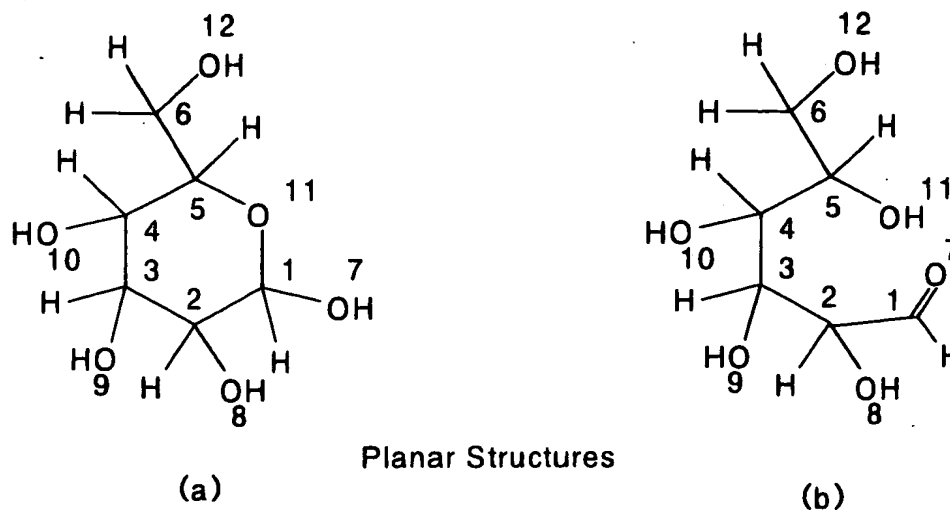


FIG. 13

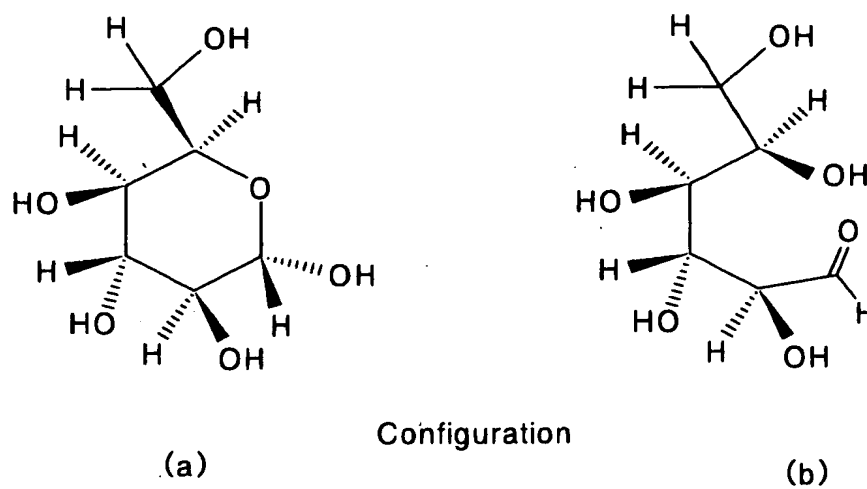
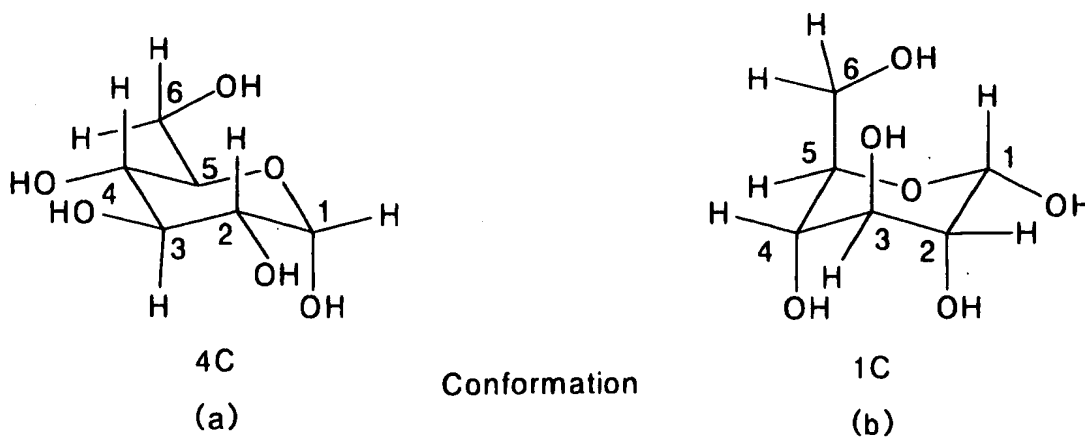


FIG. 14

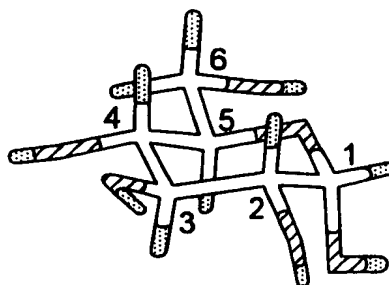


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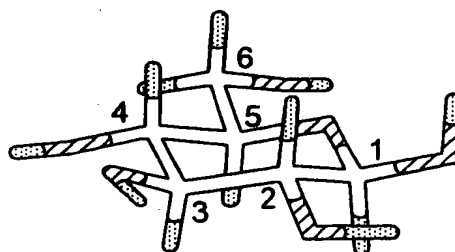
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FIG. 15

(a)

 α -glc 4C

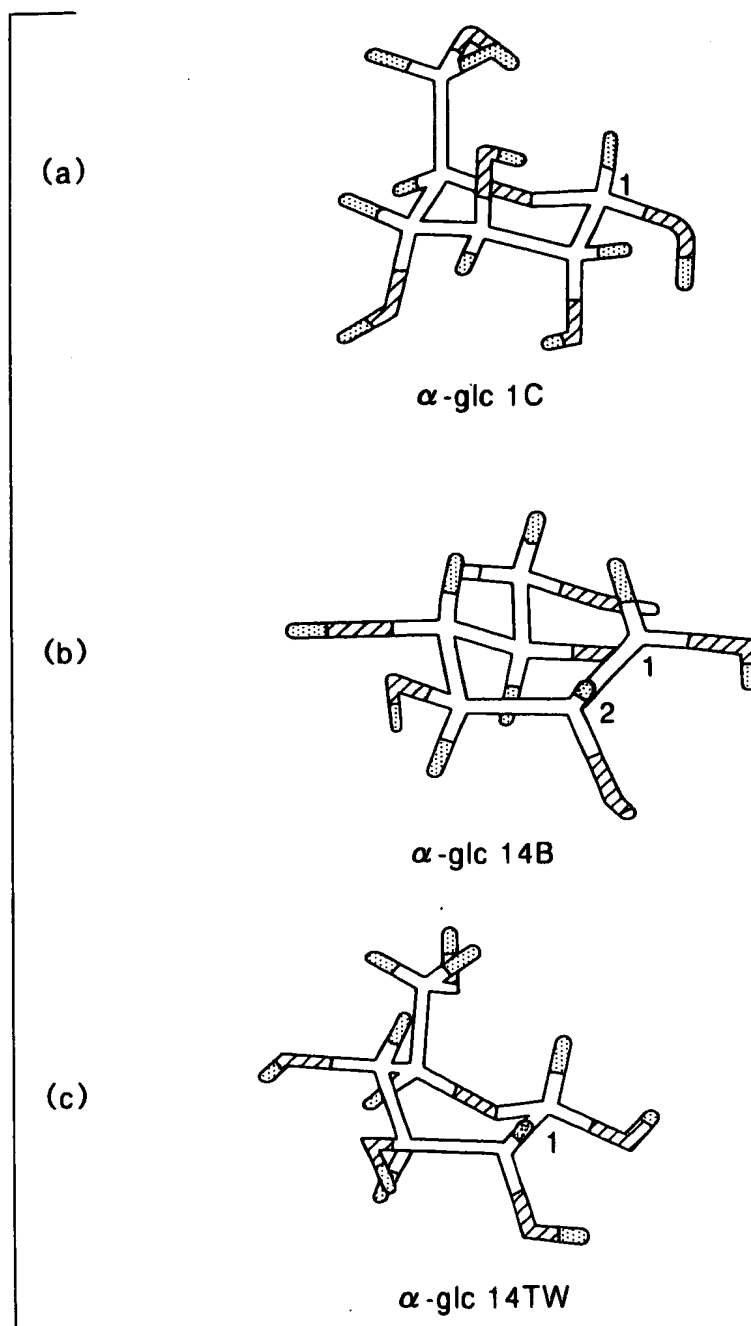
(b)

 β -glc 4C

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FIG. 16

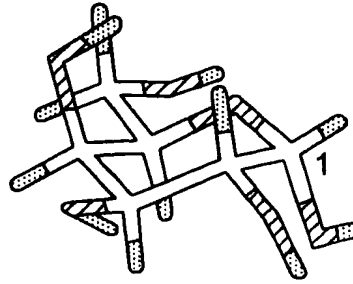


09/857610-060001

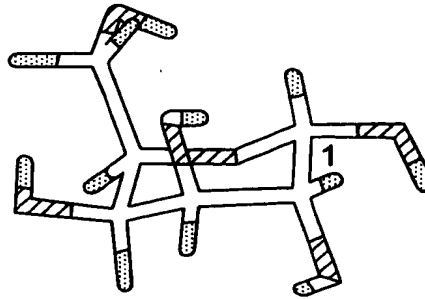
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FIG. 17

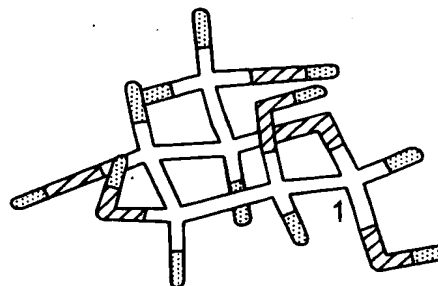
(a)

 α -gal 4C

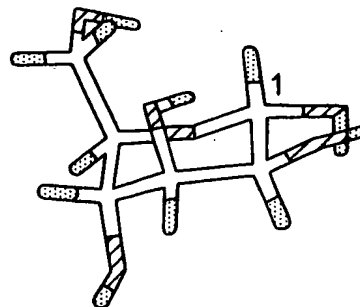
(b)

 α -gal 1C

(c)

 α -man 4C

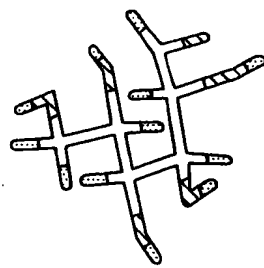
(d)

 α -man 1C

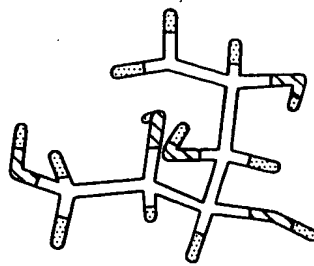
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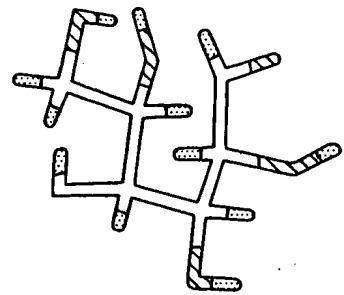
FIG. 18



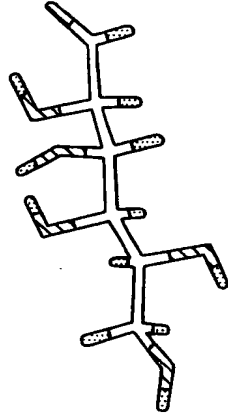
(a) α -glc 4C chain



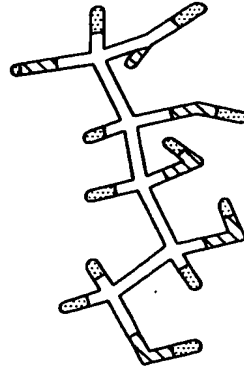
(b) α -glc 1C chain



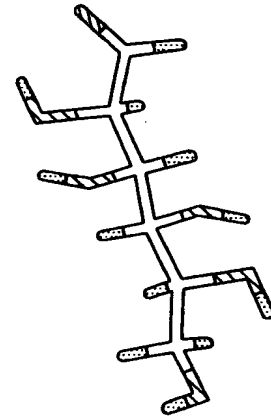
(c) α -gal 4C chain



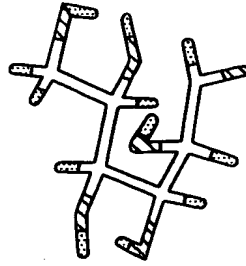
(d) α -glc 4C chain_linear



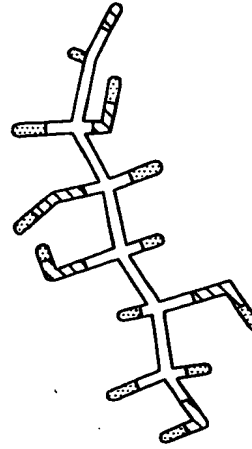
(e) α -glc 1C chain_H-bond



(f) α -gal 4C chain_linear



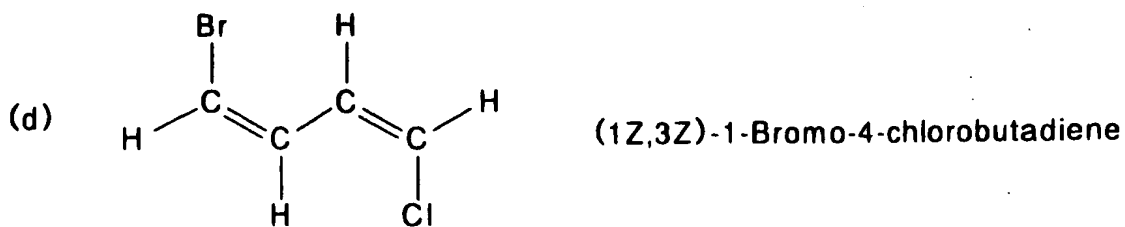
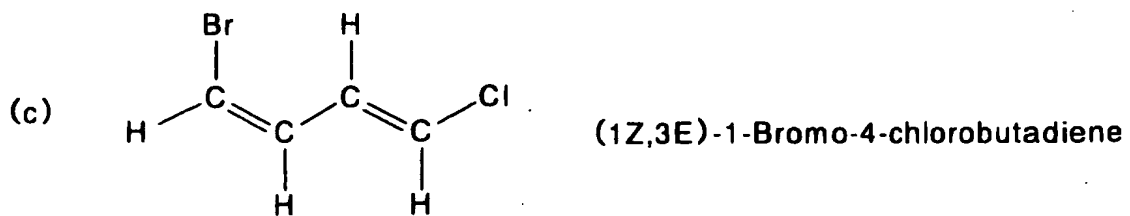
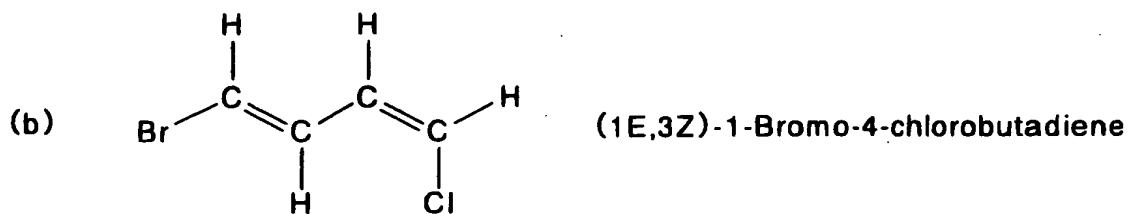
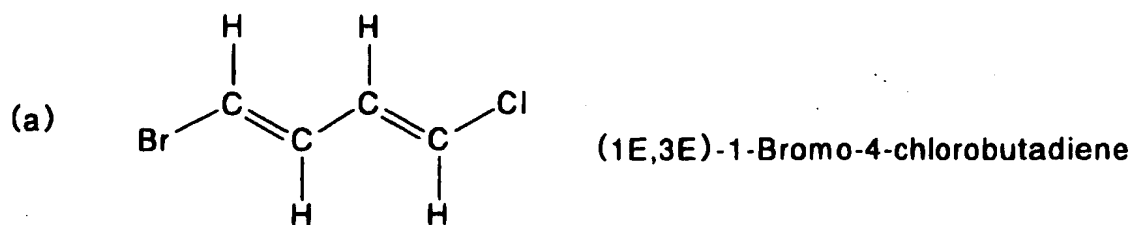
(g) α -man 4C chain



(h) α -man 4C chain_linear

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FIG. 19



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FIG. 20

a-Glc-4C

CANOST

- 1 C1*C1;Q;Q1:H*C1;Q1:H,C1,H,*C1;Q1:H,H,,&1;C2:H,*&1;Q1:H,H,,Q1:H,H,*H,,H,,*
- 2 C1*C1;C1;Q1:H*C1;Q1:H,Q;Q1:H,H,*C1;Q1:H,H,,&1,H,*&1;C2:H,H,,*,Q1:H,H,*H,,*
- 3 C1*C1;C1;Q1:H*C1;Q1:H,C1;Q1:H,H,*C2;Q;H,H,,&1;Q1:H,H,*Q1:H,H,&1,,,H,*H,,,*
- 4 C1*C1;C1;Q1:H*C1;Q1:H,C2;Q;H,H,*C1;Q1:H,H,,Q1:H,H,&1,,*&1;Q1:H,H,,H,,*,H,,,*
- 5 C1*C1;C2;Q;H*C1;Q1:H,Q1:H;H,C1,*C1;Q1:H,H,H,,&1;Q1:H*&1;Q1:H,H,,,,H,*H,,,*
- 6 C2*C1;Q1:H;H*C1;Q;H,H,,*,C1;Q1:H,C1,,*C1;Q1:H,H,,&1;Q1:H*&1;Q1:H,H,,,,H,*H,,,*
- 7 Q1*C1;H*C1;Q;H,*C1;Q1:H,C1,*C1;Q1:H,H,,&1;C2:H*&1;Q1:H,H,,Q1:H,H,*H,,H,,*
- 8 Q1*C1;H*C1;C1:H,*C1;Q1:H,Q;Q1:H,*C1;Q1:H,H,,&1,H,*&1;C2:H,H,,*,Q1:H;H,*H,,*
- 9 Q1*C1;H*C1;C1:H,*C1;Q1:H,C1;Q1;H,*C2;Q;H,H,,&1;Q1:H,H,*Q1:H;H,&1,,,H,*H,,,*
- 10 Q1*C1;H*C1;C1:H,*C1;Q1;H,C2;Q;H,*C1;Q1;H,H,,Q1;H;H,&1,*&1;Q1;H,H,,H,,*,H,,,*
- 11 Q*C1;C1*C1;C2;H,C1;Q1:H*C1;Q1;H,Q1;H;H,,&1;Q1;H,H,*&1;Q1;H,H,H,,H,,*,H,,,*
- 12 Q1*C2;H*C1;H;H,*C1;Q;H,,*C1;Q1;H,C1,*C1;Q1;H,H,,&1;Q1;H*&1;Q1;H,H,,,,H,*H,,*

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FIG. 20-1

Stereo

- 1 A*B;B;B*B*C;C;C,C,*te;si;tw,te,,tw;si;te,&l;si;te,te,,,tw;te;si,*tw,,te,*,
- 2 A*B;B;B*B*C;C;C,C,*tw;si;te,te,te,si,,&l;si;tw,tw,,,*,si;tw;te,,*te,,*,
- 3 A*B;B;B*B*C;C;C,C,*si;te;tw,tw,,tw;te;si,tw,*si;tw;te,&l,,,si,,*te,,,,*
- 4 A*B;B;B*B*C;C;C,C,*te;si;tw,si,,si;tw;te,tw,&l;te;si,tw,,te,,,*,si,,,*,
- 5 A*B;B;B*B*C;C;C,C,*tw;si;te,si,,te,te;tw;si*&l;si;tw,si,,,tw,*tw,,*,
- 6 A*B;B;B*B*C;C;C,C,,*si;tw;te,si,,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*tw,,*,
- 7 A*B;B*C;C;C,*te;tw;si,tw,*te;si;tw,te,,tw;si;te*&l;si;te,te,,,tw;te;si,*tw,,te,*,
- 8 A*B;B*C;C;C,*si;tw;te,si;tw;te,*tw;si;te,te,,te,si,&l;si;tw,tw,,,*,si;tw;te,,*te,,*,
- 9 A*B;B*C;C;C,*si;te;tw,si;tw;te,*si;te;tw,tw,,tw;te;si,tw,*si;tw;te,&l,,,si,,*te,,,,*
- 10 A*B;B*C;C;C,*si;te;tw,tw;si;te,*te;si;tw,si,,si;tw;te,tw,&l;te;si,tw,,te,,,*,si,,,*,
- 11 A*B;B*C;C;C,C,*te;si;tw,tw;te;si,,tw;si;te,tw,&l;si;te,si,,te,,,te,,*,si,,,*,
- 12 A*B;B*C;C;C,*si;tw;te,,*si;tw;te,si,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*tw,,*,

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FIG. 20-2

Configuration

- 1 A*B;B;B*B*C;C;C,C,*si;tw;te,si,,si;te;tw,*si;te;tw,si,,,si;tw;te,*si,,,si,*
- 2 A*B;B;B*B*C;C;C,C,*si;te;tw,si,,si,si,,*si;tw;te,si,,,*,si;tw;te,*si,,,*
- 3 A*B;B;B*B*C;C;C,C,*si;te;tw,si,,si;tw;te,si,,*si;tw;te,&l,,,si,,*si,,,*,
- 4 A*B;B;B*B*C;C;C,C,*si;tw;te,si,,si;tw;te,si,,*si;tw;te,si,,,*,si,,,*,
- 5 A*B;B;B*B*C;C;C,C,*si;te;tw,si,,si,,,si;te;tw*si;tw;te,si,,,*,si,,,*,
- 6 A*B;B;B*B*C;C;C,C,*si;tw;te,si,,*si;te;tw,si,,si;te;tw*si;tw;te,si,,,*,si,,,*,
- 7 A*B;B*B*C;C,*si;te;tw,si,*si;tw;te,si,,si;te;tw*si;te;tw,si,,,si;tw;te,*si,,,si,,,*
- 8 A*B;B*B*C;C,*si;tw;te,si;tw;te,*si;te;tw,si,,si,si,*si;tw;te,si,,,*,si;tw;te,*si,,,*
- 9 A*B;B*B*C;C,*si;te;tw,si;tw;te,*si;te;tw,si,,si;tw;te,si,*si;tw;te,&l,,,si,,,*,
- 10 A*B;B*B*C;C,*si;te;tw,*si;tw;te,si,,si;tw;te,si,*si;tw;te,si,,,si,,,*,si,,,*,
- 11 A*B;B*B*C;C,C,*si;tw;te,si;tw;te,,si;te;tw,si,*si;te;tw,si,,si,,,*,si,,,*,
- 12 A*B;B*B*C;C,*si;tw;te,,*si;tw;te,si,*si;te;tw,si,,si;te;tw*si;tw;te,si,,,*,si,,,*,

FIG. 21

a-glc-4C

Stereo

- 1 A*B;B;B*B*C;C;C,C,*te;si;tw,te,,tw;si;te,&l;si;te,te,,,tw;te;si,*,tw,,,te,,*
- 2 A*B;B;B;B*B*C;C;C,C,C,*tw;si;te,te,,te,si,,&l;si;tw,tw,,,*,si;tw;te,,*te,,*
- 3 A*B;B;B;B*B*C;C;C,C,C,*si;te;tw,tw,,tw;te;si,tw,,*si;tw;te,&l,,,,si,,,te,,,*
- 4 A*B;B;B;B*B*C;C;C,C,C,*te;si;tw,si,,si;tw;te,tw,,&l;te;si,tw,,,te,,,*,si,,,*
- 5 A*B;B;B;B*B*C;C;C,C,C,*tw;si;te,si,,te,,,te;tw;si*&l;si;tw,si,,,,tw,*,tw,,,*
- 6 A*B;B;B;B*B*C;C;C,C,,*si;tw;te,si,,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*,tw,,,*
- 7 A*B;B*B*C;C;C,*te;tw;si,tw,*te;si;tw,te,,tw;si;te*&l;si;te,te,,,tw;te;si,*,tw,,,te,,*
- 8 A*B;B*B*C;C;C,*si;tw;te,si;tw;te,*tw;si;te,te,,te,si,&l;si;tw,tw,,,*,si;tw;te,,*te,,*
- 9 A*B;B*B*C;C;C,*si;te;tw,si;tw;te,*si;te;tw,tw,,tw;te;si,tw,*si;tw;te,&l,,,,si,,,te,,,*
- 10 A*B;B*B*C;C;C,*si;te;tw,tw;si;te,*te;si;tw,si,,si;tw;te,tw,&l;te;si,tw,,,te,,,*,si,,,*
- 11 A*B;B*B*C;C;C,C,C,*te;si;tw,tw;te;si,,tw;si;te,tw,&l;si;te,si,,te,,,te,,,*,si,,,*
- 12 A*B;B*B*C;C;C,*si;tw;te,,*si;tw;te,si,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*,tw,,,*

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FIG. 21-1

a-glC-4C

Stereo (CH₂→H)

- 1 A*B;B;B;B*C;C;C,C,*te;si;tw,te,,tw;si;te,&l;si;te,te,,,tw;H;H,*tw,,,te,,*
- 2 A*B;B;B;B*C;C;C,C,C,*tw;si;te,te,si,,&l;si;tw,tw,,,*,si;H;H,*te,,*
- 3 A*B;B;B;B*C;C;C,C,C,*si;te;tw,tw,tw;te;si,tw,,*si;H;H,&l,,,,si,,,*,te,,,*
- 4 A*B;B;B;B*C;C;C,C,C,*te;si;tw,si,,si;H;H,tw,,&l;te;si,tw,,,te,,,*,si,,,*
- 5 A*B;B;B;B*C;C;C,C,C,*tw;si;te,si,,te,,,te;tw;si*&l;si;tw,si,,,,tw,*tw,,,*
- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*tw,,,*
- 7 A*B;B;B;B*C;C;C,*te;tw;si,tw,*te;si;tw,te,,tw;si;te*&l;si;te,te,,,tw;H;H,*tw,,,te,,*
- 8 A*B;B;B;B*C;C;C,*si;tw;te,si;tw;te,*tw;si;te,te,si,&l;si;tw,tw,,,*,si;H;H,*te,,*
- 9 A*B;B;B;B*C;C;C,*si;te;tw,si;tw;te,*si;te;tw,tw,,tw;te;si,tw,*si;H;H,&l,,,,si,,,*,te,,,*
- 10 A*B;B;B;B*C;C;C,*si;te;tw,tw;si;te,*te;si;tw,si,,si;H;H,tw,*&l;te;si,tw,,,te,,,*,si,,,*
- 11 A*B;B;B;B*C;C;C,*te;si;tw,tw;H;H,,tw;si;te,tw,*&l;si;te,si,,te,,,*,si,,,*,te,,,*
- 12 A*B;B;B;B*C;C;C,*si;tw;te,,*si;tw;te,si,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*tw,,,*

FIG. 21-2

a-Glc-4C

Stereo(CH₂→H, OH→OH)

- 1 A*B;B;B;B*C;C;C;C,*te;si;tw,OH,,tw;si;te,&l;si;te,OH,,tw;H;H,*OH,,OH,,*
- 2 A*B;B;B;B*C;C;C;C;C,*tw;si;te,OH,,te,OH,,&l;si;tw,OH,,*,si;H;H,*OH,,*
- 3 A*B;B;B;B*C;C;C;C;C,*si;te;tw,OH,,tw;te;si,OH,,*si;H;H,&l,,*,OH,,*,OH,,*,*
- 4 A*B;B;B;B*C;C;C;C;C,*te;si;tw,OH,,si;H;H,tw,,&l;te;si,OH,,*,OH,,*,*
- 5 A*B;B;B;B*C;C;C;C;C,*tw;si;te,OH,,OH,,te;tw;si*&l;si;tw,OH,,*,OH,,*,*
- 6 A*B;B;B;B*C;C;C;C,*si;tw;te,si,,*tw;si;te,OH,,te;tw;si*&l;si;tw,OH,,*,OH,,*,*
- 7 A*B;B;B;B*C;C;C,*te;tw;si,OH,*te;si;tw,te,,tw;si;te*&l;si;te,OH,,*,tw;H;H,*OH,,*,*
- 8 A*B;B;B;B*C;C;C,*si;tw;te,si;tw;te,*tw;si;te,OH,,te,OH,&l;si;tw,OH,,*,si;H;H,*OH,,*
- 9 A*B;B;B;B*C;C;C,*si;te;tw,si;tw;te,*si;te;tw,OH,,tw;te;si,OH,*si;H;H,&l,,*,OH,,*,*
- 10 A*B;B;B;B*C;C;C,*si;te;tw,tw;si;te,*te;si;tw,OH,,si;H;H,tw,&l;te;si,OH,,*,OH,,*,*
- 11 A*B;B;B;B*C;C;C;C,*te;si;tw,tw;H;H,,tw;si;te,OH,&l;si;te,OH,,*,OH,,*,*
- 12 A*B;B;B;B*C;C;C,*si;tw;te,,*si;tw;te,si,*tw;si;te,OH,,te;tw;si*&l;si;tw,OH,,*,OH,,*,*

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FIG. 22

b-Glc-4C

Stereo

- 1 A*B;B;B*B;C;C;C,C,*te;si;tw,tw,,tw;si;te,&l;si;te,te,,,tw;si:te,*tw,,,te,,*
- 2 A*B;B;B*B;C;C;C;C,C,*tw;si;te,te,te,ni,&l;si;tw,tw,,,*,si;te:tw,*te,,*
- 3 A*B;B;B*B;C;C;C;C,C,*si;te;tw,tw,,tw;si:te,si,*si;te:tw&l,,,ni,,*te,,,*
- 4 A*B;B;B*B;C;C;C;C,C,*te;si;tw,si,,si;te:tw,tw,,&l;si:te,si,,te,,,*,ni,,*,*
- 5 A*B;B;B*B;C;C;C;C,C,*tw;si;te,si,,te,,,te;si:tw&l;si;tw,si,,,on,*si,,,*
- 6 A*B;B;B*B;C;C;C;C,C,*si;tw;te,si,,*tw;si;te,si,,te;si:tw&l;si;tw,si,,,on,*si,,,*
- 7 A*B;B*B;C;C,*si:te:tw,si,*te;si;tw,tw,tw;si;te*&l;si;te,te,,,tw;si:te,*tw,,,te,,*
- 8 A*B;B*B;C;C,*si;tw;te,si;te:tw,*tw;si;te,te,,te,ni,&l;si;tw,tw,,,*,si;te:tw,*te,,*
- 9 A*B;B*B;C;C,*si;te;tw,si;tw;te,*si;te;tw,tw,,tw;si:te,si,*si;te:tw&l,,,ni,,*te,,,*
- 10 A*B;B*B;C;C,*si;te;tw,tw;si;te,*te;si;tw,si,,si;te:tw,tw,&l;si:te,si,,te,,,*,ni,,*,*
- 11 A*B;B*B;C;C;C;C,*te;si;tw,tw;si:te,,tw;si;te,te,te,te,,,tw,,,*,si,,,*,*
- 12 A*B;B*B;C;C,*si;tw;te,,*si;tw;te,si,*tw;si;te,si,,te;si:tw&l;si;tw,si,,,on,*si,,,*

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FIG. 22-1

b-Glc-4C

Stereo (CH₂→H)

- 1 A*B;B;B;B*C;C;C,C,*te;si;tw,tw,tw;si;te,&l;si;te,te,,,tw;H;H,*tw,,,te,*,
- 2 A*B;B;B;B*C;C;C,C,C,*tw;si;te,te,te,ni,,&l;si;tw,tw,,,*,si;H;H,*te,*,
- 3 A*B;B;B;B*C;C;C,C,C,*si;te;tw,tw,tw;si;te,si,,*si;H;H,&l,,,ni,,*te,,,*,
- 4 A*B;B;B;B*C;C;C,C,C,*te;si;tw,si,,si;H;H,tw,,&l;si;te,si,,,te,,,*,ni,,,*,
- 5 A*B;B;B;B*C;C;C,C,C,*tw;si;te,si,,te,,,te;si;tw*&l;si;tw,si,,,,on,*si,,,*,
- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*tw;si;te,si,,te;si;tw*&l;si;tw,si,,,,on,*si,,,*,
- 7 A*B;B;B;B*C;C,C,*si;te;tw,si,*te;si;tw,tw,tw;si;te*&l;si;te,te,,,tw;H;H,*tw,,,te,,,*,
- 8 A*B;B;B;B*C;C,C,*si;tw;te,si;te;tw,*tw;si;te,te,te,ni,&l;si;tw,tw,,,*,si;H;H,*te,,,*,
- 9 A*B;B;B;B*C;C,C,*si;te;tw,si;tw;te,*si;te;tw,tw,tw;si;te,si,*si;H;H,&l,,,ni,,*te,,,*,
- 10 A*B;B;B;B*C;C,C,*si;te;tw,tw;si;te,*te;si;tw,si,,si;H;H,tw,&l;si;te,si,,,te,,,*,ni,,,*,
- 11 A*B;B;B;B*C;C;C,C,*te;si;tw,tw;H;H,,tw;si;te,ni,&l;si;te,si,,,te,,,*,si,,,*,
- 12 A*B;B;B;B*C;C,C,*si;tw;te,,*si;tw;te,si,*tw;si;te,si,,te;si;tw*&l;si;tw,si,,,,on,*si,,,*,

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FIG. 22-2

b-Glc-4C

Stereo(CH₂→H, OH→OH)

- 1 A*B;B;B;B*C;C;C,C,*te;si;tw,OH,,tw;si;te,*&l;si;te,OH,,tw;H;H,*OH,,OH,*,*
- 2 A*B;B;B;B*C;C;C;C,C,*tw;si;te,OH,,te,OH,*&l;si;tw,OH,,*,*si;H;H,*OH,*,*
- 3 A*B;B;B;B*C;C;C;C,C,*si;te;tw,OH,,tw;si;te,OH,,*si;H;H,&l,,OH,,*OH,,*,*
- 4 A*B;B;B;B*C;C;C;C,C,*te;si;tw,OH,,si;H;H,tw,*&l;si;te,OH,,*,*OH,,*,*
- 5 A*B;B;B;B*C;C;C;C,C,*tw;si;te,OH,,te;si;tw*&l;si;tw,OH,,OH,*,*OH,,*,*
- 6 A*B;B;B;B*C;C;C,C,*si;tw;te,si,,*tw;si;te,OH,,te;si;tw*&l;si;tw,OH,,OH,*,*OH,,*,*
- 7 A*B;B;B;B*C;C,C,*si;te;tw,OH,*te;si;tw,tw,tw;si;te*&l;si;te,OH,,tw;H;H,*OH,,OH,*,*
- 8 A*B;B;B;B*C;C,C,*si;tw;te,si;te;tw,*tw;si;te,OH,,te,OH,*&l;si;tw,OH,,*,*si;H;H,*OH,,*,*
- 9 A*B;B;B;B*C;C,C,*si;te;tw,si;tw;te,*si;te;tw,OH,,tw;si;te,OH,*si;H;H,&l,,OH,,*OH,,*,*
- 10 A*B;B;B;B*C;C,C,*si;te;tw,tw;si;te,*te;si;tw,OH,,si;H;H,tw,*&l;si;te,OH,,OH,,*,*OH,,*,*
- 11 A*B;B;B;B*C;C;C,C,*te;si;tw,tw;H;H,,tw;si;te,OH,*&l;si;te,OH,,OH,,*,*OH,,*,*
- 12 A*B;B;B;B*C;C,C,*si;tw;te,,*si;tw;te,si,*tw;si;te,OH,,te;si;tw*&l;si;tw,OH,,OH,*,*OH,,*,*

FIG. 23

Comparison of a-Glc-4C with Stereo Code

a-Glc-4C

Stereo

6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*tw,,,*
 7 A*B;B;B;B*C;C;C,*te;tw;si,tw,*te;si;tw,te,,tw;si;te*&l;si;te,te,,,tw;te;si,*tw,,,te,,*

a-Glc-1C

Stereo

6 A*B;B;B;B;B*C;C;C,C,,*te;si;tw,tw,,*te;tw;si,si,,tw;si;te*&l;te;si,si,,,ni,*tw,,,*
 7 A*B;B;B;B;B*C;C;C,*si;te;tw,si,*tw;te;si,te,,te;tw;si*&l;tw;si,te,,,tw;te;si,*tw,,,te,,*

a-Glc-14B

Stereo

6 A*B;B;B;B;B*C;C;C,C,,*si;tw;te,fo,,*tw;si;te,si,,tw;si;te*&l;ei;fo,si,,,ni,*tw,,,*
 7 A*B;B;B;B;B*C;C;C,*si;te;tw,si,*ze;ei;fo,te,,ze;fo;ei*&l;si;te,te,,,tw;te;si,*tw,,,te,,*

FIG. 23-1

Stereo

6 A*B;B;B:B*C;C;C,,*se:th:el:th,,*tw:si:te;si,,*tw,*fi,,*
7 A*B;B*C;C;C,*el:th:si,*el:se:th:on,*el:th:se;si,*te,*tw:te;si,*on,*si,*

Stereo

6 A*B:B;B;B*C:C;C,C,,#si:tw;te,si,,#tw;si:te,si,,te;si:tw&l;si:tw,si,,,on,*si,,,*

7 A*B;B*C:C;C,C,*si:te:tw,si,,#te;si:tw,tw,si:te&l;si:te,te,,,tw;si:te,*tw,,,te,*,

Stereo

6 A*B;B;B;B;C;C;C,, #si;te;tw,si,, #tw;si;te,te,te;tw;si*&l;si;tw,si,,, tw,*tw,,, *

7 A*B;B;C;C;C,*te;tw;si,tw,*te;si;tw,te,,tw;si;te*&l;te;si,te,,, tw;si;te,*tw,,, te,*

FIG. 23-2

a-Gal-1C

Stereo

6 A*B;B;B*B*C;C;C,,*te:tw:si,tw,,*te:tw:si,ni,,tw:si:te*&l;te:si,si,,,ni,*th,,,*
7 A*B;B*B*C;C;C,*si:te:tw,si,*tw:te:si,te,,te:tw:si*&l;si;tw,te,,,tw:si:te,*on,,,el,,*

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a-Man-4C

Stereo

6 A*B;B;B*B*C;C;C,,*si:tw:te,si,,*tw:si:te,si,,te:tw:si*&l;tw:si,ni,,,tw,*si,,,*
7 A*B;B*B*C;C;C,*te:si:tw,tw,*te:si:tw,te,,tw:si:te*&l;si:te,on,,,tw:si:te,*tw,,,te,,*

a-Man-1C

Stereo

6 A*B;B;B*B*C;C;C,,*te:si:tw,tw,,*te:tw:si,si,,tw:si:te*&l;si:te,si,,,el,*si,,,*
7 A*B;B*B*C;C;C,*si:tw:te,si,*tw:te:si,te,,te:tw:si*&l;tw:si,te,,,tw:si:te,*tw,,,te,,*

Comparison of a-Glc-4C with Stereo Code (CH₂→H, OH→OH) FIG. 24

a-Glc-4C

StereoCH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*tw;si;te,OH,,te;tw;si*&l;si;tw,OH,,,,OH,*OH,,,*
- 7 A*B;B;B;B*C;C;C,*te;tw;si,OH,*te;si;tw,te,,tw;si;te*&l;si;te,OH,,,,tw;H;H,*OH,,OH,,*

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a-Glc-1C

StereoCH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*te;si;tw,tw,,*te;tw;si,OH,,tw;si;te*&l;te;si,OH,,,,OH,*OH,,,*
- 7 A*B;B;B;B*C;C;C,*si;te;tw,OH,*tw;te;si,te,,te;tw;si*&l;tw;si,OH,,,,tw;H;H,*OH,,OH,,*

a-Glc-14B

StereoCH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,fo,,*tw;si;te,OH,,tw;si;te*&l;ei;fo,OH,,,,OH,*OH,,,*
- 7 A*B;B;B;B*C;C;C,*si;te;tw,OH,*ze;ei;fo,te,,ze;fo;ei*&l;si;te,OH,,,,tw;H;H,*OH,,OH,,*

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FIG. 24-1

a-Glc-14TB

StereoCH2→H, OH→OH)

6 A*B;B;B;B*C;C;C,,*se:th:el:th,,*tw:si;te,OH,,tw:si;te*&l;se:th,OH,,,OH,*OH,,*

7 A*B;B;B;B*C;C,*se:el:th,OH,*el:se:th,on,el:th:se*&l;si;te,OH,,tw;H;H,*OH,,OH,*

b-Glc-4C

StereoCH2→H, OH→OH)

6 A*B;B;B;B*C;C;C,*si;tw:te,si,,*tw:si;te,OH,,te;si;tw*&l;si;tw,OH,,OH,*OH,,*

7 A*B;B;B;B*C;C,*si;te:tw,OH,*te;si;tw,tw,,tw;si;te*&l;si;te,OH,,tw;H;H,*OH,,OH,*

a-Gal-4C

StereoCH2→H, OH→OH)

6 A*B;B;B;B*C;C;C,*si;te:tw,si,,*tw:si;te,OH,,te;tw;si*&l;si;tw,OH,,OH,*OH,,*

7 A*B;B;B;B*C;C,*te;tw;si,OH,*te;si;tw,te,,tw;si;te*&l;te;si,OH,,tw;H;H,*OH,,OH,*

FIG. 24-2

a-Gal-1C

StereoCH2→H, OH→OH)

6 A*B;B;B;B*C;C;C,C,,*te:tw:si,tw,*te:tw:si,OH,,tw:si:te*&l:te:si,OH,,,OH,*,OH,,,*

7 A*B;B;B;B*C;C;C,*si:te:tw,OH,*tw:te:si,te,,te:tw:si*&l:si:tw,OH,,,tw:H;H,*,OH,,,OH,,,*

a-Man-4C

StereoCH2→H, OH→OH)

6 A*B;B;B;B*C;C;C,C,*si:tw:te,si,*tw:si:te,OH,,te;tw:si*&l:tw:si,OH,,,OH,*,OH,,,*

7 A*B;B;B;B*C;C;C,*te:si:tw,OH,*te:si:tw,te,,tw;si:te*&l:si:te,OH,,,tw:H;H,*,OH,,,OH,,,*

a-Man-1C

StereoCH2→H, OH→OH)

6 A*B;B;B;B*C;C;C,C,*te:si:tw,tw,*te:tw:si,OH,,tw:si:te*&l:si:te,OH,,,OH,*,OH,,,*

7 A*B;B;B;B*C;C;C,*si:tw:te,OH,*tw:te:si,te,,te:tw:si*&l:tw:si,OH,,,tw:H;H,*,OH,,,OH,,,*

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FIG. 25

Comparison of a-Glc-4C with Configuration Code

a-Glc-4C

Configuration

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,si;te;tw*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*C;C;C,*si;te;tw,si,*si;tw;te,si,,si;te;tw*si;te;tw,si,,,si;tw;te,*si,,,si,,*

a-Glc-1C

Configuration

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,si;te;tw*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*C;C;C,*si;te;tw,si,*si;tw;te,si,,si;te;tw*si;te;tw,si,,,si;tw;te,*si,,,si,,*

a-Glc-14B

Configuration

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,si;te;tw*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*C;C;C,*si;te;tw,si,*si;tw;te,si,,si;te;tw*si;te;tw,si,,,si;tw;te,*si,,,si,,*

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FIG. 25-1

a-Glc-14TB

Configuration

- 6 A*B;B;B*B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,*si;te;tw*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*B*C;C;C,*si;te;tw,si,*si;tw;te,si,,*si;te;tw*si;te;tw,si,,,si;tw;te,*si,,,si,,*

b-Glc-4C

Configuration

- 6 A*B;B;B;B*B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,*si;tw;te*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*B*C;C;C,*si;te;tw,si,*si;tw;te,si,,*si;te;tw*si;te;tw,si,,,si;te;tw,*si,,,si,,*

a-Gal-4C

Configuration

- 6 A*B;B;B;B*B*C;C;C,C,,*si;te;tw,si,,*si;te;tw,si,,*si;te;tw*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*B*C;C;C,*si;te;tw,si,*si;tw;te,si,,*si;te;tw*si;tw;te,si,,,si;te;tw,*si,,,si,,*

FIG. 25-2

a-Gal-1C

Configuration

- 6 A*B;B;B;B*C;C;C,C,,*si;te;tw,si,,*si;te;tw,si,,*si;te;tw*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*C;C;C,*si;te;tw,si,*si;tw;te,si,,*si;te;tw*si;tw;te,si,,,si;te;tw,*si,,,si,,,*

a-Man-4C

Configuration

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,*si;te;tw*si;te;tw,si,,,si,*si,,,*
- 7 A*B;B*C;C;C,*si;tw;te,si,*si;tw;te,si,,*si;te;tw*si;te;tw,si,,,si;te;tw,*si,,,si,,,*

a-Man-1C

Configuration

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,*si;te;tw*si;te;tw,si,,,si,*si,,,*
- 7 A*B;B*C;C;C,*si;tw;te,si,*si;tw;te,si,,*si;te;tw*si;te;tw,si,,,si;te;tw,*si,,,si,,,*

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FIG. 26

Comparison of a-Glc-4C-chain with Stereo Code

a-Glc-4C-chain

Stereo

- 6 A*B;B;B*B*C;C;C,C,,*si;tw;te,te,,*tw;si;te,si,,*te;si;tw,si,,*te;fi,th,,*
- 7 A*B*C;C*te;tw;si,*te;si;tw,el,*tw;si;te,te,,*si;te;tw,tw,,*si;tw;te,si,,*si,,,*

a-Glc-4C-chain-linear

Stereo

- 6 A*B;B;B*B*C;C;C,C,,*si;tw;te,te,,*si;te;tw,si,,*si;tw;te,te,,*se;tw,fi,,*
- 7 A*B*C;C*se;ze;th,*si;tw;te,te,*,*si;te;tw,si,,*si;te;tw,tw,,*si;tw;te,si,,*si,,,*

a-Glc-1C-chain

Stereo

- 6 A*B;B;B*B*C;C;C,C,,*te;si;tw,ni,,*te;tw;si,si,,*tw;te;si,si,,*si;tw,tw,,*
- 7 A*B*C;C*si;te;tw,*tw;te;si,te,*te;tw;si,te,,*te;tw;si,tw,,*si;tw;te,fo,,*te,,,*

FIG. 26-1

a-Glc-1C-chain-Hbond

Stereo

- 6 A*B;B;B*B*C;C;C,C,,*te:si:tw,tw,,*si:te:tw,se,,*tw:te:si,el,,*ni:th,fo,,*
- 7 A*B*C;C*ni:on:fi,*tw:te:si,ze,*si:te:tw,th,,*te:tw:si,th,,*si:tw:te,te,*el,,,*

a-Gal-4C-chain

Stereo

- 6 A*B;B;B*B*C;C;C,C,,*si:te:tw,el,,*tw:si:te,te,,*te:si:tw,si,,*te:fi,th,,*
- 7 A*B*C;C*te:tw:si,*te:si:tw,te,*tw:te:si,te,,*si:te:tw,tw,,*si:tw:te,si,,*tw,,,*

a-Gal-4C-chain-linear

Stereo

- 6 A*B;B;B*B*C;C;C,C,,*si:te:tw,te,,*si:te:tw,el,,*si:tw:te,ni,,*ei:tw,fi,,*
- 7 A*B*C;C*ei:ze:fo,*si:tw:te,on,*si:tw:te,on,,*si:te:tw,th,,*si:tw:te,si,,*tw,,,*

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FIG. 26-2

a-Man-4C-chain

Stereo

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,el,,*tw;si;te,si,,*te;tw;si,ni,,*te;fi,si,,*
- 7 A*B*C;C*te;si;tw,*te;si;tw,te,*tw;si;te,on,,*si;te;tw,tw,,*si;tw;te,se,,*tw,,,*

a-Man-4C-chain-linear

Stereo

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,el,,*si;te;tw,se,,*se;el;th,el,,*fo;te,ei,,*
- 7 A*B*C;C*fo;ze;ei,se;th;el,ze,*si;te;tw,th,,*si;te;tw,th,,*si;tw;te,si,,*tw,,,*

CANOST

- 6 C2*C1;Q1;H;H*C1;Q1;H,H,,*C1;Q1;H,H,,*V1;Q1;H,H,,*QD;H,H,,*
- 7 QD*V1*C1;H*C1;Q1;H,*C1;Q1;H,H,*C1;Q1;H,H,,*Q1;H;H,H,,*H,,,*

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FIG. 27

Comparison of α -Glc-4C-chain with Stereo Code (CH₂→H, OH→OH)

α -Glc-4C-chain

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,,*si;tw;te,OH,,*tw;si;te,OH,,*te;si;tw,OH,,*te;fi,OH,,*
- 7 A*B*C;C*te;tw;si,*te;si;tw,OH,*tw;si;te,OH,,*si;te;tw,OH,,*si;H;H,OH,,*OH,,*,

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α -Glc-4C-chain-linear

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,,*si;tw;te,OH,,*si;te:tw,OH,,*si:tw;te,OH,,*se:tw,OH,,*
- 7 A*B*C;C*se:ze:th,*si:tw:te,OH,*si:te:tw,OH,,*si;te;tw,OH,,*si;H;H,OH,,*OH,,*,

α -Glc-1C-chain

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,,*te:si:tw,OH,,*te:tw:si,OH,,*tw:te:si,OH,,*si:tw,OH,,*
- 7 A*B*C;C*si:te:tw,*tw:te:si,OH,*te:tw:si,OH,,*te:tw:si,OH,,*si;H;H,OH,,*OH,,*,

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FIG. 27-1

a-Glc-1C-chain-Hbond

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*te:si:tw,OH,,*si:te:tw,OH,,*tw:te:si,OH,,*ni:th,OH,,*
- 7 A*B*C;C*ni:on:fi,*tw:te:si,OH,*si:te:tw,OH,,*te:tw:si,OH,,*si;H;H,OH,,*OH,,,*

a-Gal-4C-chain

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*si;te:tw,OH,,*tw;si;te,OH,,*te;si;tw,OH,,*te;fi,OH,,*
- 7 A*B*C;C*te;tw;si,*te;si;tw,OH,*tw:te:si,OH,,*si;te;tw,OH,,*si;H;H,OH,,*OH,,,*

a-Gal-4C-chain-linear

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*si;te:tw,OH,,*si:te:tw,OH,,*si:tw:te,OH,,*ei:tw,OH,,*
- 7 A*B*C;C*ei:ze:fo,*si:tw:te,OH,*si:tw:te,OH,,*si;te;tw,OH,,*si;H;H,OH,,*OH,,,*

FIG. 27-2

a-Man-4C-chain

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,OH,,*tw;si;te,OH,,*te;tw;si,OH,,*te;fi,OH,,*
- 7 A*B*C;C*te;si;tw,*te;si;tw,OH,*tw;si;te,OH,,*si;te;tw,OH,,*si;H;H,OH,,*OH,,,*

a-Man-4C-chain-linear

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,OH,,*si;te;tw,OH,,*se;el;th,OH,,*fo;te,OH,,*
- 7 A*B*C;C*fo;ze;ei,*se;th;el,OH,*si;te;tw,OH,,*si;te;tw,OH,,*si;H;H,OH,,*OH,,,*

CANOST

- 6 C2*C1;Q1;H;H*C1;Q1;H,H,,*C1;Q1;H,H,,*V1;Q1;H,H,,*QD;H,H,,*
- 7 QD*V1*C1;H*C1;Q1;H,*C1;Q1;H,H,*C1;Q1;H,H,,*C2;Q1;H,H,,*Q1;H;H,H,*H,,,*

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FIG. 28

Comparison of a-Glc-4C-chain with Configuration Code

a-Glc-4C-chain

Configuration

- 6 A*B;B;B:B*C;C;C,C,,*si;tw;te,si,,*si;tw;te,si,,*si;ze,si,,*
- 7 A*B*C;C*si;te;tw,*si;tw;te,si,*si;te;tw,si,,*si;tw;te,si,,*si,,*

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a-Glc-4C-chain-linear

Configuration

- 6 A*B;B;B:B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,*si;tw;te,si,,*si;ze,si,,*
- 7 A*B*C;C*si;te;tw,*si;tw;te,si,*si;te;tw,si,,*si;tw;te,si,,*si,,*

a-Glc-1C-chain

Configuration

- 6 A*B;B;B:B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,*si;tw;te,si,,*si;ze,si,,*
- 7 A*B*C;C*si;te;tw,*si;tw;te,si,*si;te;tw,si,,*si;tw;te,si,,*si,,*

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FIG. 28-1

a-Glc-1C-chain-Hbond

Configuration

- 6 A*B:B;B;B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,*si;tw;te,si,,*si;ze,si,,*
- 7 A*B*C;C*si;te;tw,*si;tw;te,si,*si;te;tw,si,,*si;te;tw,si,,*si;tw;te,si,,*si,,,*

a-Gal-4C-chain

Configuration

- 6 A*B:B;B;B*C;C;C,C,,*si;te;tw,si,,*si;te;tw,si,,*si;tw;te,si,,*si;ze,si,,*
- 7 A*B*C;C*si;te;tw,*si;tw;te,si,*si;tw;te,si,,*si;te;tw,si,,*si;tw;te,si,,*si,,,*

a-Gal-4C-chain-linear

Configuration

- 6 A*B:B;B;B*C;C;C,C,,*si;te;tw,si,,*si;te;tw,si,,*si;tw;te,si,,*si;ze,si,,*
- 7 A*B*C;C*si;te;tw,*si;tw;te,si,*si;tw;te,si,,*si;te;tw,si,,*si;tw;te,si,,*si,,,*

FIG. 28-2

a-Man-4C-chain

Configuration

- 6 A*B;B;B;B*C;C;C,,*si;tw;te,si,,*si;te;tw,si,,*si;te;tw,si,,*si;ze,si,,*
- 7 A*B*C;C*si;tw;te,*si;tw;te,si,*si;te;tw,si,,*si;te;tw,si,,*si;tw;te,si,,*si,,*

a-Man-4C-chain-linear

Configuration

- 6 A*B;B;B;B*C;C;C,,*si;tw;te,si,,*si;te;tw,si,,*si;te;tw,si,,*si;ze,si,,*
- 7 A*B*C;C*si;tw;te,*si;tw;te,si,*si;te;tw,si,,*si;te;tw,si,,*si;tw;te,si,,*si,,*

CANOST

- 6 C2*C1;Q1;H;H*C1;Q1;H,H,,*C1;Q1;H,H,,*V1;Q1;H,H,,*QD;H,H,,*
- 7 QD*V1*C1;H*C1;Q1;H,*C1;Q1;H,H,*C1;Q1;H,H,,*C2;Q1;H,H,,*Q1;H;H,H,,*H,,*

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FIG. 29

Comparison of 1Br4Cl_butadiene isoers

CANOST

Br LB*D1*D1;H*D1;H,*D1;H,*LC;H,*

Cl LC*D1*D1;H*D1;H,*D1;H,*LB;H,*

1E3E1Br4Cl_butadiene

Stereo

Br A*B*C;C*si;ze,*si;ze,*si;ze,*

Cl A*B*C;C*si;ze,*si;ze,*si;ze,*

Configuration

Br A*B*C;C*si;ze,*si;ze,*si;ze,*

Cl A*B*C;C*si;ze,*si;ze,*si;ze,*

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1E3Z1Br4Cl_butadiene FIG. 29-1

Stereo

Br A*B*C;C*si;ze,*si;ze,*ze;si,*Cl A*B*C;C*ze;si,*si;ze,*si;ze, *

Configuration

Br A*B*C;C*si;ze,*si;ze,*ze;si,*Cl A*B*C;C*ze;si,*si;ze,*si;ze, *

1Z3E1Br4Cl_butadiene

Stereo

Br A*B*C;C*ze;si,*si;ze,*si;ze, *Cl A*B*C;C*si;ze,*si;ze,*ze;si,*

Configuration

Br A*B*C;C*ze;si,*si;ze,*si;ze, *Cl A*B*C;C*si;ze,*si;ze,*ze;si,*

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FIG. 29-2

1Z3Z1Br4Cl_butadiene

Stereo

Br A*B*C;C*ze;si,*si;ze,*ze;si,*Cl A*B*C;C*ze;si,*si;ze,*ze;si,*

Configuration

Br A*B*C;C*ze;si,*si;ze,*ze;si,*Cl A*B*C;C*ze;si,*si;ze,*ze;si,*

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FIG. 30

